Linear Scaling Nanoscience Simulation for Petascale Computing: the 3D Fragment Method

NCCS USERS MEETING

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Project Overview

- **The project participants:**

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- **Briefly summary:**

  It calculates the electronic structures of 10,000 atom nano structures using LS3DF method, especially it studies the internal electric field effects in such nanosystems.

- **Project milestones:**

  (1) To run the LS3DF code on jaguar for tens of thousands of processes.

  (2) To study the total dipole moments of CdSe quantum dots for different dot size, surface passivation, and crystal structures.

  (2) To study the internal electric field for ZnO/ZnS core shell structures.

  (3) To study the ZnOTe alloys, the feasibility of using such material for solar cell applications.

Project impact

- **Understand the internal electric field of nanostructures.**

  The internal electric field is an unsolved problem in nanoscience due to difficulty to experimentally probe it.

  The internal electric field can significantly alter the electronic structure, optical properties, and carrier dynamics.

- **A better understanding of this problem can help us to design better nanoscience applications, from optical probes, to solar cells.**

  It will have broad impact from nanoscience to energy science.

Previous divide-and-conquer methods

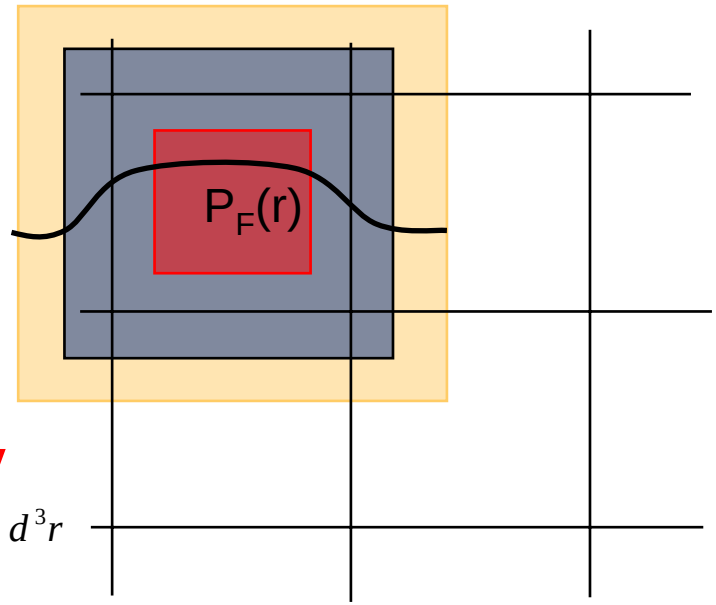
- **Using partition function $P_F(r)$:** $\sum_F P_F(r) = 1$

$$\rho_{tot}(r) = \sum_F P_F(r)\rho_F(r)$$

Center region $P_F(r) = 1$

Overlap region $P_F(r) < 1$

Buffer region $P_F(r) = 0$



- **No unique way to divide kinetic energy**

$$\sum_F \int P_F(r)\psi_F(r)\nabla^2\psi_F(r)d^3r \quad \textbf{or} \quad \sum_F \int P_F(r)\,|\nabla\psi_F(r)|^2\,d^3r$$

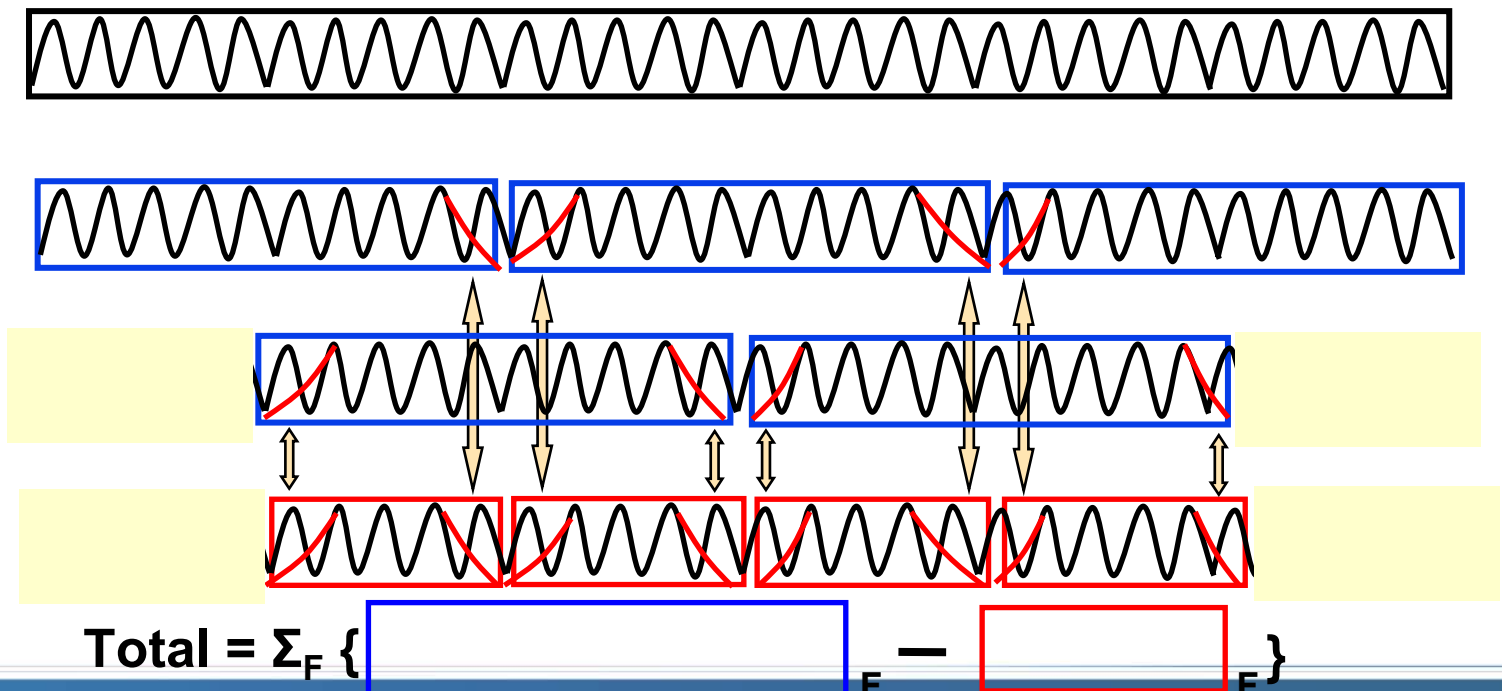
- **Require** $\rho_F(r) = \rho_{tot}(r)$ **in the overlap region**

- **Introduce additional correction terms:**
  the result is not the same as the original full system LDA

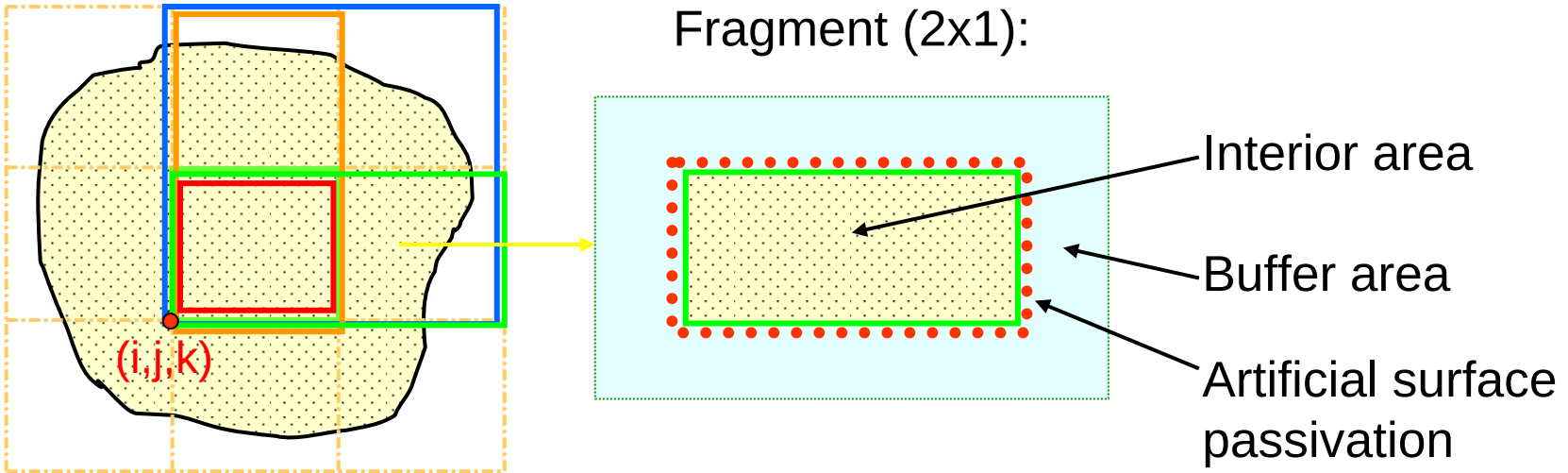
Linear scaling 3 dimensional fragment method (LS3DF)

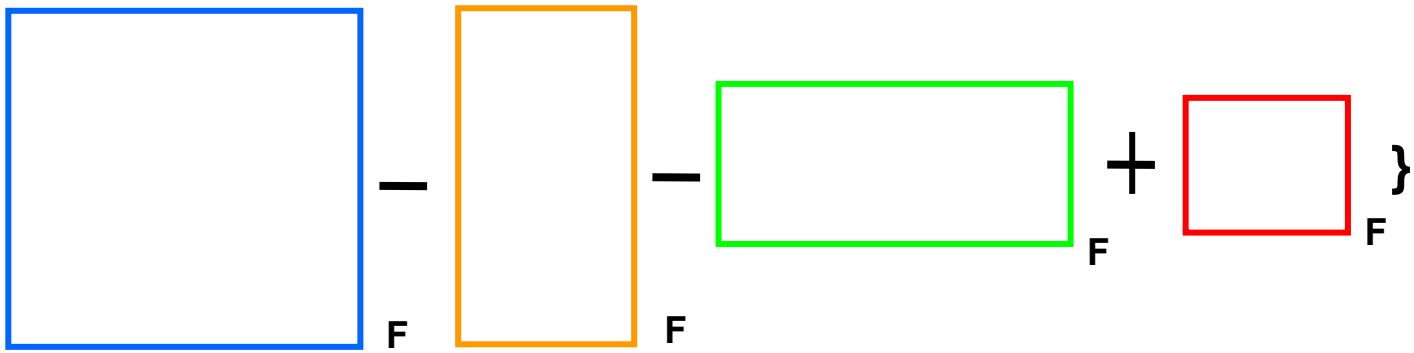
- A novel scheme for dividing and patching the space
- No spatial partition functions
- Using overlapping positive and negative pieces (fragments)
- Cancellation for the artificial boundary effects

1D example:



LS3DF (linear scaling 3D fragment) dividing and patching scheme

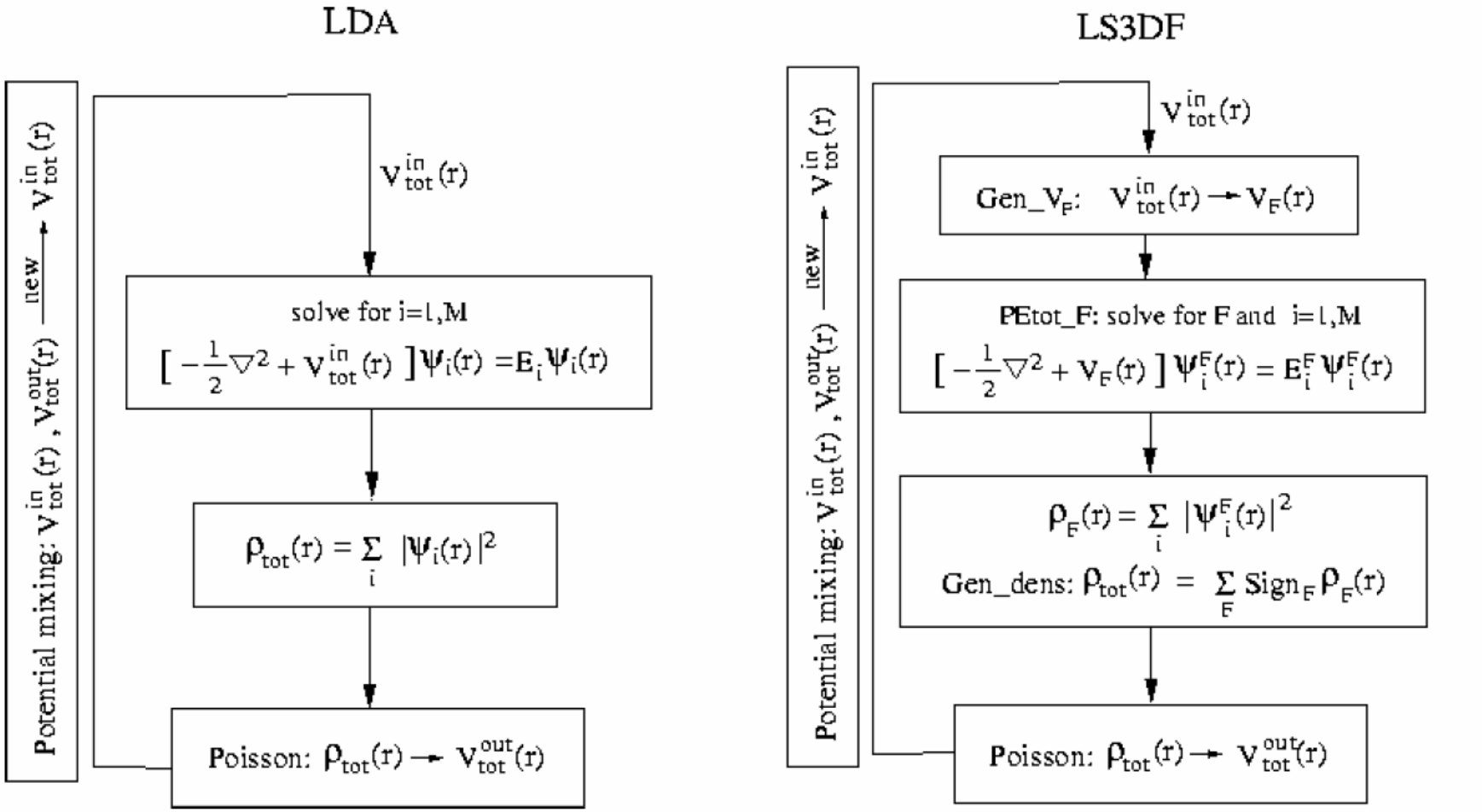


Total = Σ_F {  **}**

$$System = \sum_{i,j,k} \{F_{222} + F_{211} + F_{121} + F_{112} - F_{221} - F_{212} - F_{122} - F_{111}\}$$

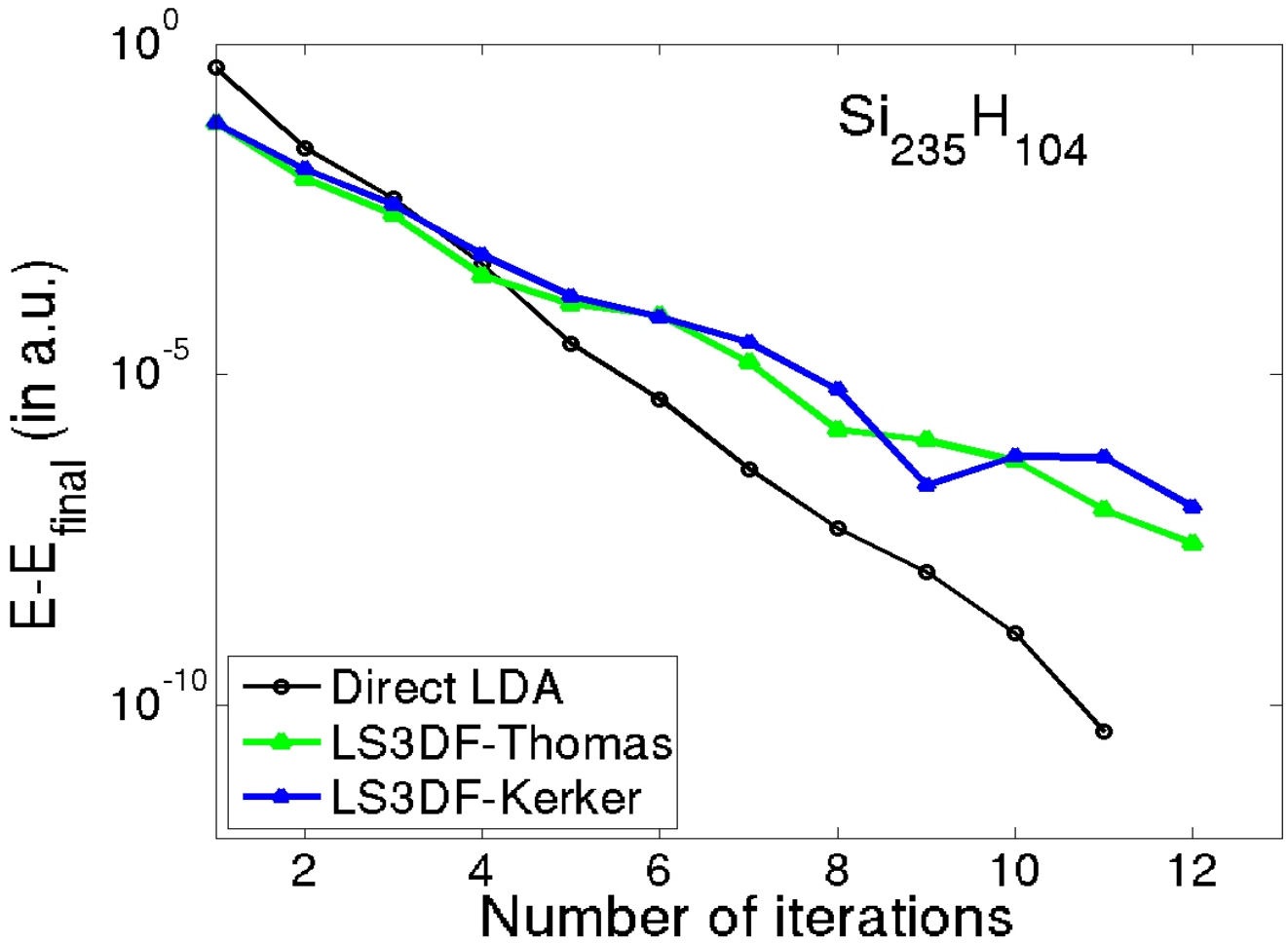
Boundary effects are cancelled out between the fragments!

Flow chart of LS3DF



The code is based on PEtot; each group of processors (e.g, 16) solves one fragment, then the fragments are patched back together. A Poisson equation is solved for the whole system.

The convergence of LS3DF

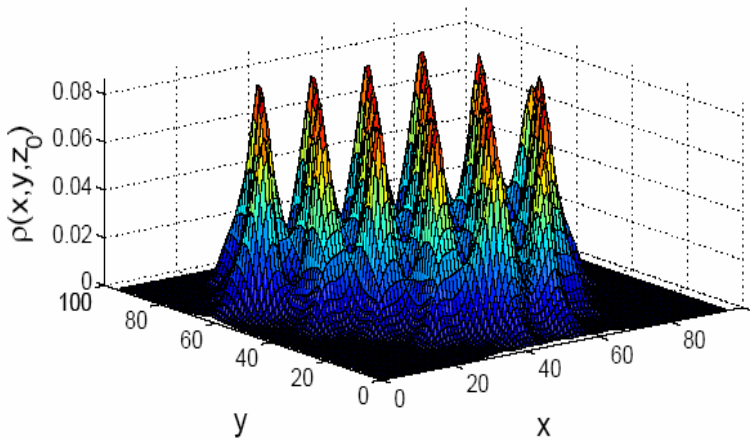


LS3DF result is essentially the same as direct LDA

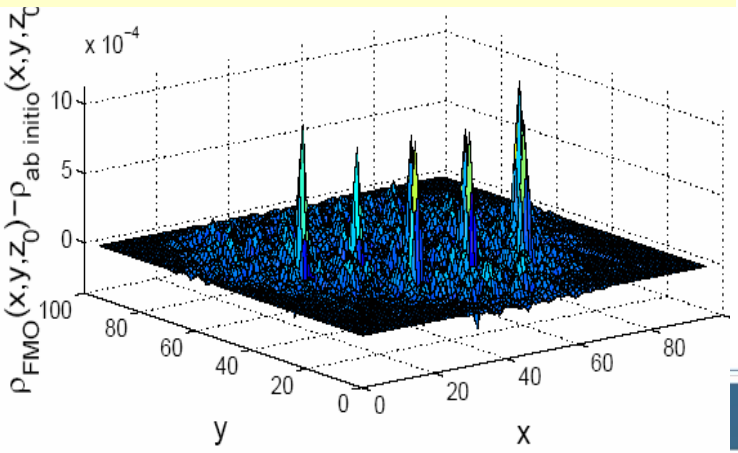
- The total energy difference: 3meV/atom ~ 0.1 kcal/mol
  (better than the typical 0.1eV error introduced by other numerical approximations: PW cut off, pseudopotential)

- Charge density difference: 0.2%

- Atomic force difference: 10^{-5} a.u
  (an order of magnitude smaller than the typical stopping criterion for atomic relaxation)



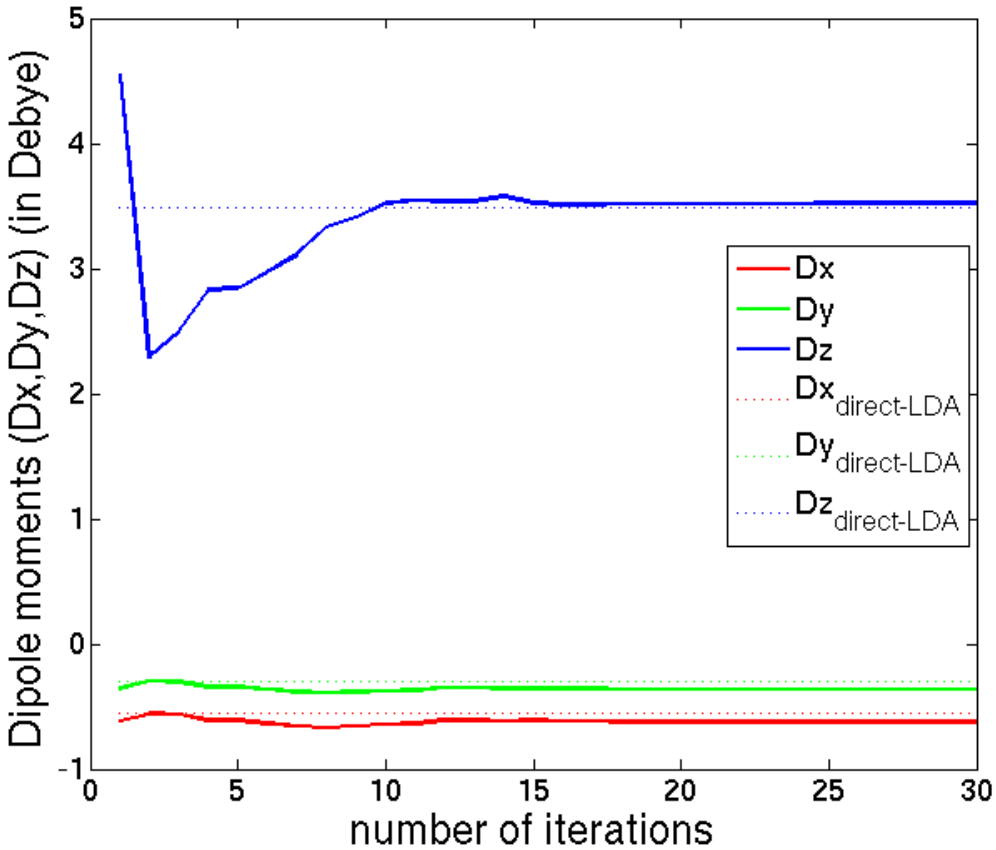
ρ



Δρ

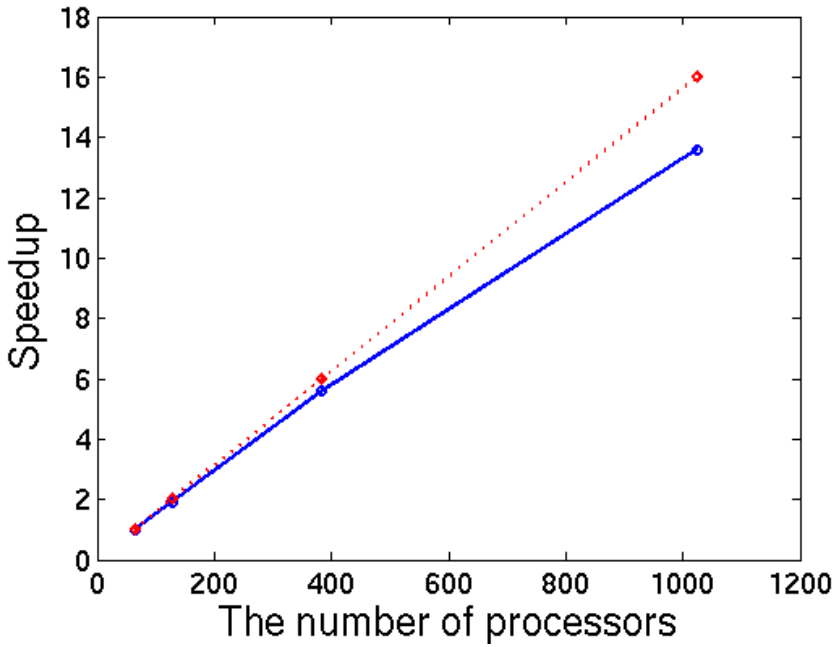
Applications of LS3DF

Dipole moment calculations of CdSe nanorod

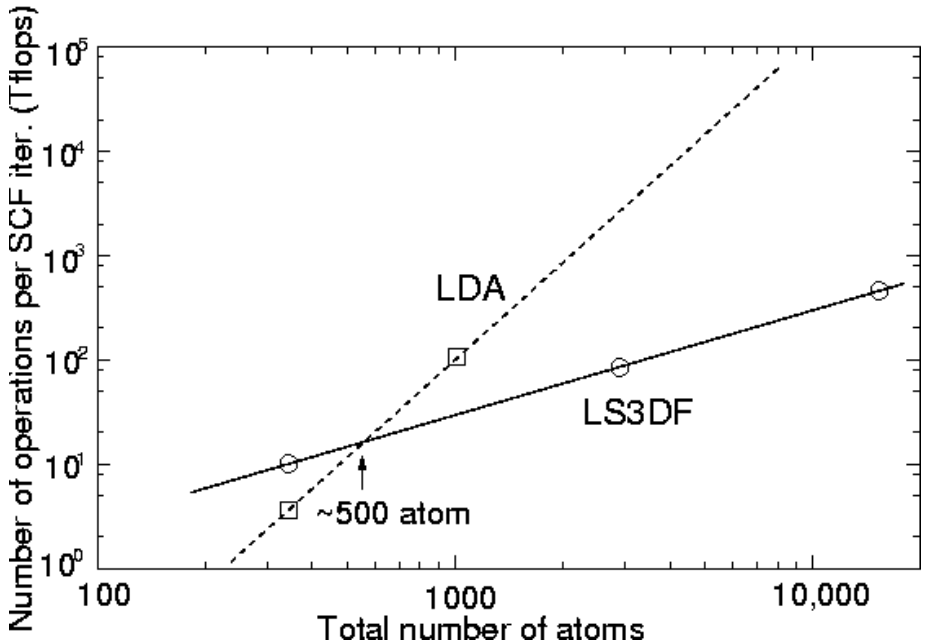


The scaling of LS3DF

LS3DF speed up (for a 3,000 atom system)

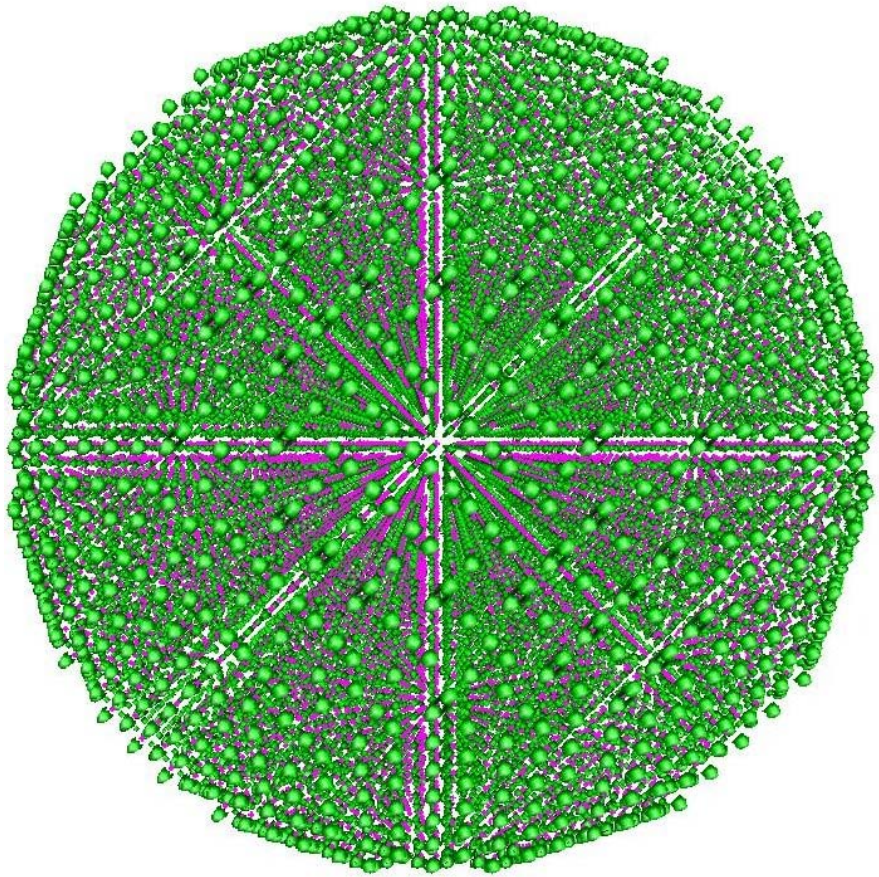


Cross over between LS3DF and direct LDA



We believe LS3DF should scale well up to >100,000 processors for ~100,000 atom systems. It is well suited for petascale computation.

15,000 atom quantum dot: $Si_{13607}H_{2236}$



Project logistics

- **What size production jobs will you be running?**

  5,000 to 10,000 cores, for 5-10 hour runs.

- **Do you have any special requirements**

  Library: (ACML) 1dfft, lapack

  Data storage: 500 GB per job, possibly thousands of files

  I/O: relatively heavy IO.

- **Do you have any special visualization needs?**

  No. Very basic visualization needs: gnuplot, gOpenmol

Project logistics (continued)

- **What development efforts are required?**

  Need to port the code to jaguar, test the performance.

  Possibly like to improve the performance of the code by doing the all-band algorithm.

  Might need to change the code, so all the wavefunctions are held in memory.

- **What issues/problems do you anticipate as you begin production?**

  Need to test the I/O, possibly eliminate it by hold the data in memory

- **What level of interaction do you anticipate with the NCCS staff?**

  We will know later. Need technical support to get start it.